

## WHAT IS CLAIMED IS:

1           1.     A spectral processing method for compensating a plurality of  
2 sequential spectra and profiles derived therefrom for effects of drift comprising:  
3           transforming a plurality of sequential spectra obtained from a spectrometer to  
4 provide an array of drift-compensated row vectors, wherein the array of drift-  
5 compensated row vectors constitutes a drift-compensated array;  
6           performing a principal-factor determination on the drift-compensated array to  
7 provide a set of drift-compensated principal factors; and  
8           generating drift-compensated scaled target-factor profiles from a profile  
9 trajectory of the drift-compensated row vectors lying within a space of drift-  
10 compensated principal factors.

1           2.     The spectral processing method of claim 1 further comprising  
2 generating drift-compensated compositional profiles from the drift-compensated  
3 scaled target-factor profiles.

1           3.     The spectral processing method of claim 1, wherein the transforming  
2 the plurality of sequential spectra further comprises:  
3           inputting a plurality of sequential spectra from a spectrometer into a computer  
4 system;  
5           ordering the spectra in a primal array of row vectors, wherein each sequential  
6 spectrum constitutes a successive row vector of the primal array; and  
7           removing phase factors due to drift using a dephasing procedure that  
8 transforms the primal array into a drift-compensated array.

1           4.     The spectral processing method of claim 3 wherein the dephasing  
2     procedure for transforming the primal array into the drift-compensated array further  
3     comprises applying a Fourier transform to the spectra in the primal array of row  
4     vectors forming an array of Fourier-transformed row vectors, multiplying each  
5     Fourier-transformed row vector by a complex conjugate of each Fourier-transformed  
6     row vector to form a squared moduli vector thereby removing phase factors due to  
7     drift, taking the square root of each element of the squared moduli vector to create a  
8     corresponding moduli vector, and forming a drift-compensated array of moduli  
9     vectors by successively sequencing the moduli vectors as successive drift-  
10    compensated row vectors in a drift-compensated array, wherein the moduli vectors  
11    constitute moduli of Fourier-transformed spectra.

1           5.     The spectral processing method of claim 4 further comprising  
2     outputting the drift-compensated row vectors of the drift-compensated array as a  
3     sequential series of moduli of Fourier-transformed spectra.

1           6.     The spectral processing method of claim 3 wherein the dephasing  
2     procedure for transforming the primal array into the drift-compensated array further  
3     comprises applying a fitting procedure to each spectrum in the primal array using  
4     selected reference spectra, calculating through the fitting procedure a corresponding  
5     reference weighting factor for each reference spectrum corresponding to each  
6     spectrum in the primal array, removing the phase factor due to drift from each  
7     spectrum in the primal array by synthesizing a corresponding drift-compensated  
8     spectrum given by the sum of each selected reference spectrum multiplied by the

9 corresponding reference weighting factor, and forming a drift-compensated array by  
10 successively sequencing the drift-compensated spectra as successive drift-  
11 compensated row vectors in the drift-compensated array.

1 7. The spectral processing method of claim 6 further comprising  
2 outputting analytical results selected from the group consisting of the selected  
3 reference spectra used in the fitting procedure, the drift-compensated row vectors of  
4 the drift-compensated array as a sequential series of drift-compensated spectra,  
5 reference weighting factors for each reference spectrum corresponding to each  
6 spectrum in the primal array as a set of drift-compensated reference-spectrum  
7 profiles, and phase factors due to drift for each reference spectrum corresponding to  
8 each spectrum in the primal array as a set of phase-factor profiles.

1 8. The spectral processing method of claim 1 wherein the performing the  
2 principal-factor determination comprises performing a factor analysis.

1 9. The spectral processing method of claim 8, wherein the performing the  
2 factor analysis further comprises:

3 forming a covariance array from the drift-compensated array;

4 applying an eigenanalysis to the covariance array to define a complete set of  
5 eigenvectors and eigenvalues; and

6 defining a set of drift-compensated principal factors by selecting a subset of  
7 eigenvectors from the complete set of eigenvectors.

1 10. The spectral processing method of claim 9, wherein the defining the

2 set of drift-compensated principal factors further comprises selecting the drift-  
3 compensated principal factors as a first few eigenvectors corresponding to  
4 eigenvalues above a certain limiting value.

1 11. The spectral processing method of claim 1 wherein the performing the  
2 principal-factor determination comprises performing a linear-least-squares analysis.

1 12. The spectral processing method of claim 11, wherein the performing a  
2 linear-least-squares analysis further comprises:

3 selecting a set of initial factors from the set of drift-compensated row vectors  
4 of the drift-compensated array;

5 performing a linear-least-squares decomposition with the set of initial factors  
6 on the drift-compensated row vectors in the drift-compensated array to provide a set  
7 of residue factors; and

8 performing a Gram-Schmidt orthonormalization on the combined set of initial  
9 factors and residue factors to provide drift-compensated principal factors.

1 13. The spectral processing method of claim 1, wherein the generating  
2 drift-compensated scaled target-factor profiles further comprises:

3 constructing a set of drift-compensated target factors on a space of the drift-  
4 compensated principal factors;

5 applying the set of drift-compensated target factors to a profile trajectory lying  
6 within a space of drift-compensated principal factors to obtain a sequential set of  
7 target-factor weighting factors corresponding to the drift-compensated target factors

8 for the profile trajectory; and  
9 outputting analytical results selected from the group consisting of a set of  
10 drift-compensated scaled target-factor profiles derived from the set of target-factor  
11 weighting factors, and the set of drift-compensated target factors.

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1 14. The spectral processing method of claim 13, wherein the constructing  
2 the set of drift-compensated target factors further comprises:

3 generating a profile trajectory on a 3-dimensional projection of a 4-  
4 dimensional space of a set of first-four, drift-compensated principal factors along  
5 with a reference tetrahedron the vertices of which represent each of the first-four,  
6 drift-compensated principal factors;

7 enclosing the profile trajectory within an enclosing tetrahedron with vertices  
8 centered on end-points and in proximity to turning points of the profile trajectory, and  
9 with faces lying essentially tangent to portions of the profile trajectory; and

10 calculating the drift-compensated target factors from the normed coordinates  
11 of the vertices of the enclosing tetrahedron in terms of the drift-compensated  
12 principal factors.

1 15. The spectral processing method of claim 14, wherein the generating  
2 the profile trajectory further comprises:

3 calculating 4-space coordinates of a profile trajectory of drift-compensated  
4 target-factor profiles on a 4-dimensional space to produce four coordinates for each  
5 point in the profile trajectory, one coordinate for each of the first-four, drift-  
6 compensated principal factors;

7           reducing the dimensionality of the coordinates of the profile trajectory by  
8   dividing each coordinate by a sum of all four 4-space coordinates to produce normed  
9   coordinates for the profile trajectory; and,  
10          plotting the normed coordinates for the profile trajectory in a 3-dimensional  
11   space the coordinate axes of which are edges of a reference tetrahedron, the  
12   vertices of which correspond to unit values for each of the first-four, drift-  
13   compensated principal factors in a manner analogous to plotting of coordinates on a  
14   quaternary phase diagram.

1           16.   The spectral processing method of claim 13, wherein generating drift-  
2   compensated compositional profiles comprises:  
3          defining a set of drift-compensated scaled target-factor profile values as the  
4   set of scaled target-factor weighting factors;  
5          dividing each drift-compensated scaled target-factor profile value by a profile  
6   sensitivity factor for each constituent corresponding to the target factor to provide a  
7   sensitivity-scaled target-factor profile value;  
8          normalizing the sensitivity-scaled target-factor profile value by dividing each  
9   sensitivity-scaled target-factor profile value for a given cycle number by the sum of  
10   all the sensitivity-scaled target-factor profile values for the given cycle number to  
11   provide drift-compensated compositional profile values at the given cycle number;  
12   and  
13          outputting the drift-compensated compositional profile values as a set of drift-  
14   compensated compositional profiles.

1 17. A waveform processing method for compensating a plurality of  
2 sequential waveforms and profiles derived therefrom for effects of drift comprising:  
3 transforming a plurality of sequential waveforms obtained from a waveform-  
4 source device to provide an array of drift-compensated row vectors, wherein the  
5 array of drift-compensated row vectors constitutes a drift-compensated array;  
6 performing a principal-factor determination on the drift-compensated array to  
7 provide a set of drift-compensated principal factors; and  
8 generating drift-compensated scaled target-factor profiles from a profile  
9 trajectory of the drift-compensated row vectors lying within a space of drift-  
10 compensated principal factors .  
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1 18. The waveform processing method of claim 17, wherein the  
2 transforming the plurality of sequential waveforms further comprises:  
3 inputting a plurality of sequential waveforms from a waveform-source device  
4 into a computer system;  
5 ordering the waveforms in a primal array of row vectors, wherein each  
6 sequential waveform constitutes a successive row vector of the primal array; and  
7 removing phase factors due to drift using a dephasing procedure that  
8 transforms the primal array into a drift-compensated array.  
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1 19. The waveform processing method of claim 18 wherein the dephasing  
2 procedure for transforming the primal array into the drift-compensated array further  
3 comprises applying a Fourier transform to the waveforms in the primal array of row

4 vectors forming an array of Fourier-transformed row vectors, multiplying each  
5 Fourier-transformed row vector by a complex conjugate of each Fourier-transformed  
6 row vector to form a squared moduli vector thereby removing phase factors due to  
7 drift, taking the square root of each element of the squared moduli vector to create a  
8 corresponding moduli vector, and forming a drift-compensated array of moduli  
9 vectors by successively sequencing the moduli vectors as successive drift-  
10 compensated row vectors in a drift-compensated array, wherein the moduli vectors  
11 constitute moduli of Fourier-transformed waveforms.

1 20. The waveform processing method of claim 19 further comprising  
2 outputting the drift-compensated row vectors of the drift-compensated array as a  
3 sequential series of moduli of Fourier-transformed waveforms.

1 21. The waveform processing method of claim 18, wherein the dephasing  
2 procedure for transforming the primal array into the drift-compensated array further  
3 comprises applying a fitting procedure to each sequential waveform in the primal  
4 array using selected reference waveforms, calculating through the fitting procedure a  
5 corresponding reference weighting factor for each reference waveform  
6 corresponding to each waveform in the primal array, removing the phase factor due  
7 to drift from each waveform in the primal array by synthesizing a corresponding drift-  
8 compensated waveform given by the sum of each selected reference waveform  
9 multiplied by the corresponding reference weighting factor, and forming a drift-  
10 compensated array by successively sequencing the drift-compensated waveforms  
11 as successive drift-compensated row vectors in the drift-compensated array.



1           22.    The waveform processing method of claim 21 further comprising  
2    outputting analytical results selected from the group consisting of the selected  
3    reference waveforms used in the fitting procedure, the drift-compensated row  
4    vectors of the drift-compensated array as a sequential series of drift-compensated  
5    waveforms, reference weighting factors for each reference waveform corresponding  
6    to each waveform in the primal array as a set of drift-compensated reference-  
7    waveform profiles, and phase factors due to drift for each reference waveform  
8    corresponding to each waveform in the primal array as a set of phase-factor profiles.

1           23.    The waveform processing method of claim 17 wherein the performing  
2    the principal-factor determination comprises performing a factor analysis.

1           24.    The waveform processing method of claim 23, wherein the performing  
2    the factor analysis further comprises:

3               forming a covariance array from the drift-compensated array;

4               applying an eigenanalysis to the covariance array to define a complete set of  
5    eigenvectors and eigenvalues; and

6               defining a set of drift-compensated principal factors by selecting a subset of  
7    eigenvectors from the complete set of eigenvectors.

1           25.    The waveform processing method of claim 24, wherein the defining the  
2    set of drift-compensated principal factors further comprises selecting the drift-  
3    compensated principal factors as a first few eigenvectors corresponding to  
4    eigenvalues above a certain limiting value.

1           26.    The waveform processing method of claim 17 wherein the performing  
2   the principal-factor determination comprises performing a linear-least-squares  
3   analysis.

1           27.    The waveform processing method of claim 26, wherein the performing  
2   a linear-least-squares analysis further comprises:

3           selecting a set of initial factors from the set of drift-compensated row vectors  
4   of the drift-compensated array;

5           performing a linear-least-squares decomposition with the set of initial factors  
6   on the drift-compensated row vectors in the drift-compensated array to provide a set  
7   of residue factors; and

8           performing a Gram-Schmidt orthonormalization on the combined set of initial  
9   factors and residue factors to provide drift-compensated principal factors.

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1           28.    The waveform processing method of claim 17, wherein the generating  
2   drift-compensated scaled target-factor profiles further comprises:

3           constructing a set of drift-compensated target factors on a space of the drift-  
4   compensated principal factors;

5           applying the set of drift-compensated target factors to a profile trajectory lying  
6   within a space of drift-compensated principal factors to obtain a sequential set of  
7   target-factor weighting factors corresponding to the drift-compensated target factors  
8   for the profile trajectory; and

9           outputting analytical results selected from the group consisting of a set of  
10   drift-compensated scaled target-factor profiles derived from the set of target-factor

11 weighting factors, and the set of drift-compensated target factors.

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1 29. The waveform processing method of claim 28, wherein the

2 constructing the set of drift-compensated target factors further comprises:

3 generating a profile trajectory on a 3-dimensional projection of a 4-

4 dimensional space of a set of first-four, drift-compensated principal factors along

5 with a reference tetrahedron the vertices of which represent each of the first-four,

6 drift-compensated principal factors;

7 enclosing the profile trajectory within an enclosing tetrahedron with vertices

8 centered on end-points and in proximity to turning points of the profile trajectory, and

9 with faces lying essentially tangent to portions of the profile trajectory; and

10 calculating the drift-compensated target factors from the normed coordinates

11 of the vertices of the enclosing tetrahedron in terms of the drift-compensated

12 principal factors.

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1 30. The waveform processing method of claim 29, wherein the generating

2 the profile trajectory further comprises:

3 calculating 4-space coordinates of a profile trajectory of drift-compensated

4 target-factor profiles on a 4-dimensional space to produce four coordinates for each

5 point in the profile trajectory, one coordinate for each of the first-four, drift-

6 compensated principal factors;

7 reducing the dimensionality of the coordinates of the profile trajectory by

8 dividing each coordinate by a sum of all four 4-space coordinates to produce normed

- 9 coordinates for the profile trajectory; and,
- 10 plotting the normed coordinates for the profile trajectory in a 3-dimensional
- 11 space the coordinate axes of which are edges of a reference tetrahedron, the
- 12 vertices of which correspond to unit values for each of the first-four, drift-
- 13 compensated principal factors in a manner analogous to plotting of coordinates on a
- 14 quaternary phase diagram.
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1           31.    An apparatus for compensating a plurality of sequential spectra and  
2    profiles derived therefrom for effects of drift comprising a spectroscopic analysis  
3    system, wherein the spectroscopic analysis system comprises:  
4           a spectrometer; and  
5           a computer system, coupled to the spectrometer, for analyzing spectra input  
6    from the spectrometer, the computer system further comprising a spectral processor  
7    for compensating a plurality of sequential spectra and profiles derived therefrom for  
8    effects of drift.

1           32.    The apparatus of claim 31, wherein the spectrometer comprises an  
2    electron spectrometer.

1           33.    The apparatus of claim 32, wherein the electron spectrometer  
2    comprises an Auger spectrometer.

1           34.    The apparatus of claim 32, wherein the electron spectrometer  
2    comprises an x-ray photoelectron spectrometer.

1           35.    The apparatus of claim 32, wherein the electron spectrometer  
2    comprises an electron energy loss spectrometer.

1           36.    The apparatus of claim 31, wherein the spectral processor further  
2 comprises:

3           a spectral transformer operating on a plurality of sequential spectra obtained  
4 from the spectrometer to provide an array of drift-compensated row vectors, wherein  
5 the array of drift-compensated row vectors constitutes a drift-compensated array;

6           a principal-factor determinator operating on the drift-compensated array to  
7 provide a set of drift-compensated principal factors; and

8           a profile generator operating on a profile trajectory of the drift-compensated  
9 row vectors lying within a space of drift-compensated principal factors to provide a  
10 set of drift-compensated scaled target-factor profiles.

1           37.    The apparatus of claim 36, wherein the profile generator operating on  
2 the set drift-compensated scaled target-factor profiles generates a set of drift-  
3 compensated compositional profiles.

1           38.    The apparatus of claim 36, wherein the spectral transformer accepts  
2 as input the plurality of sequential spectra obtained from the spectrometer into the  
3 computer system, orders the spectra in a primal array, wherein each sequential  
4 spectrum constitutes a successive row vector of the primal array, and removes  
5 phase factors due to drift using a dephasor that transforms the primal array into a  
6 drift-compensated array.

1           39.    The apparatus of claim 38, wherein the dephaser that transforms the  
2    primal array into the drift-compensated array applies a Fourier transform to the  
3    spectra in the primal array of row vectors to form an array of Fourier-transformed  
4    row vectors, multiplies each Fourier-transformed row vector by a complex conjugate  
5    of each Fourier-transformed row vector to form a squared moduli vector thereby  
6    removing phase factors due to drift, takes the square root of each element of the  
7    squared moduli vector to create a corresponding moduli vector, and forms a drift-  
8    compensated array of moduli vectors by successively sequencing the moduli vectors  
9    as successive drift-compensated row vectors in a drift-compensated array, wherein  
10   the moduli vectors constitute moduli of Fourier-transformed spectra.

1           40.    The apparatus of claim 39 wherein the spectral transformer outputs to  
2    an output device the drift-compensated row vectors of the drift-compensated array  
3    as a sequential series of moduli of Fourier-transformed spectra.

1           41.    The apparatus of claim 38, wherein the dephaser that transforms the  
2    primal array into the drift-compensated array fits each spectrum in the primal array  
3    using selected reference spectra, calculates a corresponding reference weighting  
4    factor for each reference spectrum corresponding to each spectrum in the primal  
5    array, synthesizes a corresponding drift-compensated spectrum given by the sum of  
6    each selected reference spectrum multiplied by the corresponding reference  
7    weighting factor thereby removing phase factors due to drift, and forms a drift-  
8    compensated array by successively sequencing the drift-compensated spectra as  
9    successive drift-compensated row vectors in the drift-compensated array.

1           42.    The apparatus of claim 41 wherein the spectral transformer outputs to  
2   an output device analytical results selected from the group consisting of the selected  
3   reference spectra used in the fitting procedure, the drift-compensated row vectors of  
4   the drift-compensated array as a sequential series of drift-compensated spectra,  
5   reference weighting factors for each reference spectrum corresponding to each  
6   spectrum in the primal array as a set of drift-compensated reference-spectrum  
7   profiles, and phase factors due to drift for each reference spectrum corresponding to  
8   each spectrum in the primal array as a set of phase-factor profiles.

1           43.    The apparatus of claim 36 wherein the principal-factor determinator  
2   comprises a factor analyzer.

1           44.    The apparatus of claim 43, wherein the factor analyzer forms a  
2   covariance array from the drift-compensated array, applies an eigenanalysis to the  
3   covariance array to define a complete set of eigenvectors and eigenvalues, and  
4   defines a set of drift-compensated principal factors as a subset of eigenvectors  
5   determined by a selector operating on the complete set of eigenvectors.

1           45.    The apparatus of claim 44, wherein the selector operates on the  
2   complete set of eigenvectors to define the set of drift-compensated principal factors  
3   as a first few eigenvectors corresponding to eigenvalues above a certain limiting  
4   value.

1           46.    The apparatus of claim 36 wherein the principal-factor determinator  
2   comprises a linear-least-squares analyzer.



1           47.    The apparatus of claim 46, wherein the linear-least-squares analyzer  
2   selects a set of initial factors from the set of drift-compensated row vectors of the  
3   drift-compensated array, performs a linear-least-squares decomposition with the set  
4   of initial factors on the drift-compensated row vectors in the drift-compensated array  
5   to provide a set of residue factors, and performs a Gram-Schmidt orthonormalization  
6   on the combined set of initial factors and residue factors to provide drift-  
7   compensated principal factors.

1           48.    The apparatus of claim 36, wherein the profile generator defines a set  
2   of drift-compensated target factors on a space of the drift-compensated principal  
3   factors determined by a target-factor constructor operating on the drift-compensated  
4   principal factors, applies the set of drift-compensated target factors to a profile  
5   trajectory lying within a space of drift-compensated principal factors to obtain a  
6   sequential set of target-factor weighting factors corresponding to the drift-  
7   compensated target factors for the profile trajectory, and outputs to an output device  
8   analytical results selected from the group consisting of a set of drift-compensated  
9   scaled target-factor profiles derived from the set of target-factor weighting factors,  
10   and the set of drift-compensated target factors.

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1           49.    The apparatus of claim 48, wherein the target-factor constructor generates  
2   a profile trajectory on a 3-dimensional projection of a 4-dimensional space of a set of  
3   first-four, drift-compensated principal factors along with a reference tetrahedron the  
4   vertices of which represent each of the first-four, drift-compensated principal factors;  
5   encloses the profile trajectory within an enclosing tetrahedron with vertices centered on

6 end-points and in proximity to turning points of the profile trajectory, and with faces lying  
7 essentially tangent to portions of the profile trajectory; and calculates the drift-  
8 compensated target factors from the normed coordinates of the vertices of the enclosing  
9 tetrahedron in terms of the drift-compensated principal factors.

1 50. The apparatus of claim 49, wherein the target-factor constructor in  
2 generating the profile trajectory further calculates 4-space coordinates of a profile  
3 trajectory of drift-compensated target-factor profiles on a 4-dimensional space to  
4 produce four coordinates for each point in the profile trajectory, one coordinate for  
5 each of the first-four, drift-compensated principal factors; reduces the dimensionality  
6 of the coordinates of the profile trajectory by dividing each coordinate by a sum of all  
7 four 4-space coordinates to produce normed coordinates for the profile trajectory;  
8 and, plots the normed coordinates for the profile trajectory in a 3-dimensional space  
9 the coordinate axes of which are edges of a reference tetrahedron the vertices of  
10 which correspond to unit values for each of the first-four, drift-compensated principal  
11 factors in a manner analogous to plotting of coordinates on a quaternary phase  
12 diagram.

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1 51. The apparatus of claim 48, wherein the profile generator further defines a  
2 set of drift-compensated scaled target-factor profile values as the set of scaled target-  
3 factor weighting factors, divides each drift-compensated scaled target-factor profile  
4 value by a profile sensitivity factor for each constituent corresponding to the target factor  
5 to provide a sensitivity-scaled target-factor profile value, divides each sensitivity-scaled  
6 target-factor profile value for a given cycle number by the sum of all the sensitivity-

- 7 scaled target-factor profile values for the given cycle number to provide drift-
- 8 compensated compositional profile values at the given cycle number, and outputs the
- 9 drift-compensated compositional profile values as a set of drift-compensated
- 10 compositional profiles.
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1           52.    An apparatus for compensating a plurality of sequential waveforms and  
2 profiles derived therefrom for effects of drift, comprising a waveform analysis  
3 system, wherein the waveform analysis system comprises:

4           a waveform-source device; and

5           a computer system, coupled to the waveform-source device, for analyzing  
6 waveforms input from the waveform-source device, the computer system further  
7 comprising a waveform processor for compensating a plurality of sequential  
8 waveforms and profiles derived therefrom for effects of drift.

1           53.    The apparatus of claim 52, wherein the waveform processor further  
2 comprises:

3           a waveform transformer operating on a plurality of sequential waveforms  
4 obtained from a waveform-source device to provide an array of drift-compensated  
5 row vectors, wherein the array of drift-compensated row vectors constitutes a drift-  
6 compensated array;

7           a principal-factor determinator operating on the drift-compensated array to  
8 provide a set of drift-compensated principal factors; and

9           a profile generator operating on a profile trajectory of the drift-compensated  
10 row vectors lying within a space of drift-compensated principal factors to provide a  
11 set of drift-compensated scaled target-factor profiles.

1           54.    The apparatus of claim 53, wherein the waveform transformer accepts  
2    as input the plurality of sequential waveforms obtained from a waveform-source  
3    device into the computer system, orders the waveforms in a primal array, wherein  
4    each sequential waveform constitutes a successive row vector of the primal array,  
5    and removes phase factors due to drift using a dephasor that transforms the primal  
6    array into a drift-compensated array.

1           55.    The apparatus of claim 54, wherein the dephasor that transforms the  
2    primal array into the drift-compensated array applies a Fourier transform to the  
3    primal array of row vectors to form an array of Fourier-transformed row vectors,  
4    multiplies each Fourier-transformed row vector by a complex conjugate of each  
5    Fourier-transformed row vector to form a squared moduli vector thereby removing  
6    phase factors due to drift, takes the square root of each element of the squared  
7    moduli vector to create a corresponding moduli vector, and forms a drift-  
8    compensated array of moduli vectors by successively sequencing the moduli vectors  
9    as successive drift-compensated row vectors in a drift-compensated array, wherein  
10   the moduli vectors constitute moduli of Fourier-transformed waveforms.

1           56.    The apparatus of claim 55 wherein the waveform transformer outputs  
2    the drift-compensated row vectors of the drift-compensated array as a sequential  
3    series of moduli of Fourier-transformed waveforms.

1           57.    The apparatus of claim 54, wherein the dephasor that transforms the  
2    primal array into the drift-compensated array fits each waveform in the primal array  
3    using selected reference waveforms, calculates a corresponding reference weighting  
4    factor for each reference waveform corresponding to each waveform in the primal  
5    array, synthesizes a corresponding drift-compensated waveform given by the sum of  
6    each selected reference waveform multiplied by the corresponding reference  
7    weighting factor thereby removing phase factors due to drift, and forms a drift-  
8    compensated array by successively sequencing the drift-compensated waveforms  
9    as successive drift-compensated row vectors in the drift-compensated array.

1           58.    The apparatus of claim 57 wherein the waveform transformer outputs  
2    to an output device analytical results selected from the group consisting of the  
3    selected reference waveforms used in the fitting procedure, the drift-compensated  
4    row vectors of the drift-compensated array as a sequential series of drift-  
5    compensated waveforms, reference weighting factors for each reference waveform  
6    corresponding to each waveform in the primal array as a set of drift-compensated  
7    reference-waveform profiles, and phase factors due to drift for each reference  
8    waveform corresponding to each waveform in the primal array as a set of phase-  
9    factor profiles.

1           59.    The apparatus of claim 53 wherein the principal-factor determinator  
2    comprises a factor analyzer.

1           60.    The apparatus of claim 59, wherein the factor analyzer forms a  
2   covariance array from the drift-compensated array, applies an eigenanalysis to the  
3   covariance array to define a complete set of eigenvectors and eigenvalues, and  
4   defines a set of drift-compensated principal factors as a subset of eigenvectors  
5   determined by a selector operating on the complete set of eigenvectors.

1           61.    The apparatus of claim 60, wherein the selector operates on the  
2   complete set of eigenvectors to define the set of drift-compensated principal factors  
3   as a first few eigenvectors corresponding to eigenvalues above a certain limiting  
4   value.

1           62.    The apparatus of claim 53 wherein the principal-factor determinator  
2   comprises a linear-least-squares analyzer.

1           63.    The apparatus of claim 62, wherein the linear-least-squares analyzer  
2   selects a set of initial factors from the set of drift-compensated row vectors of the  
3   drift-compensated array, performs a linear-least-squares decomposition with the set  
4   of initial factors on the drift-compensated row vectors in the drift-compensated array  
5   to provide a set of residue factors, and performs a Gram-Schmidt orthonormalization  
6   on the combined set of initial factors and residue factors to provide drift-  
7   compensated principal factors.

1           64.    The apparatus of claim 53, wherein the profile generator defines a set  
2   of drift-compensated target factors on a space of the drift-compensated principal  
3   factors determined by a target-factor constructor operating on the drift-compensated

4 principal factors, applies the set of drift-compensated target factors to a profile  
 5 trajectory lying within a space of drift-compensated principal factors to obtain a  
 6 sequential set of target-factor weighting factors corresponding to the drift-  
 7 compensated target factors for the profile trajectory, and outputs to an output device  
 8 analytical results selected from the group consisting of a set of drift-compensated  
 9 scaled target-factor profiles derived from the set of target-factor weighting factors,  
 10 and the set of drift-compensated target factors.

11

65. The apparatus of claim 64, wherein the target-factor constructor generates  
 a profile trajectory on a 3-dimensional projection of a 4-dimensional space of a set of  
 first-four, drift-compensated principal factors along with a reference tetrahedron the  
 vertices of which represent each of the first-four, drift-compensated principal factors;  
 encloses the profile trajectory within an enclosing tetrahedron with vertices centered on  
 end-points and in proximity to turning points of the profile trajectory, and with faces lying  
 essentially tangent to portions of the profile trajectory; and calculates the drift-  
 compensated target factors from the normed coordinates of the vertices of the enclosing  
 tetrahedron in terms of the drift-compensated principal factors.

66. The apparatus of claim 65, wherein the target-factor constructor in  
 generating the profile trajectory further calculates 4-space coordinates of a profile  
 trajectory of drift-compensated target-factor profiles on a 4-dimensional space to  
 produce four coordinates for each point in the profile trajectory, one coordinate for each  
 of the first-four, drift-compensated principal factors; reduces the dimensionality of the  
 coordinates of the profile trajectory by dividing each coordinate by a sum of all four 4-



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1           67.    An article of manufacture comprising a program storage medium readable  
2 by a computer, the medium tangibly embodying one or more programs of instructions  
3 executable by the computer to perform a method for compensating a plurality of  
4 sequential spectra and profiles derived therefrom for effects of drift, the method  
5 comprising:

6           transforming a plurality of sequential spectra obtained from a spectrometer to  
7 provide an array of drift-compensated row vectors, wherein the array of drift-  
8 compensated row vectors constitutes a drift-compensated array;

9           performing a principal-factor determination on the drift-compensated array to  
10 provide a set of drift-compensated principal factors; and,

11           generating drift-compensated scaled target-factor profiles from a profile trajectory  
12 of the drift-compensated row vectors lying within a space of drift-compensated principal  
13 factors.

1           68.    The article of manufacture comprising a program storage medium  
2 readable by a computer, the medium tangibly embodying one or more programs of  
3 instructions executable by the computer to perform a method for compensating a  
4 plurality of sequential spectra and profiles derived therefrom for effects of drift, the  
5 method of claim 67 further comprising generating drift-compensated compositional  
6 profiles from the set of drift-compensated scaled target-factor profiles.

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1           69.    An article of manufacture comprising a program storage medium readable  
2 by a computer, the medium tangibly embodying one or more programs of instructions  
3 executable by the computer to perform a method for compensating a plurality of  
4 sequential waveforms and profiles derived therefrom for effects of drift, the method  
5 comprising:

6           transforming a plurality of sequential waveforms obtained from a waveform-  
7 source device to provide an array of drift-compensated row vectors, wherein the array of  
8 drift-compensated row vectors constitutes a drift-compensated array;

9           performing a principal-factor determination on the drift-compensated array to  
10 provide a set of drift-compensated principal factors; and,

11           generating drift-compensated scaled target-factor profiles from a profile trajectory  
12 of the drift-compensated row vectors lying within a space of drift-compensated principal  
13 factors.